What is principal component analysis?

May 26, 2014 in education, expository | Tags: affine space, factor analysis, Jeopardy!, least squares, low rank approximation, maximum likelihood, MDS, multi-dimensional scaling, PCA, pPCA, principal component analysis, probabilistic PCA, Pythagoras' theorem, regression, Schoenberg's theorem, singular value decomposition

In the ***Jeopardy!*** game show contestants are presented with questions formulated as answers that require answers in the form questions. For example, if a contestant selects "Normality for $200″ she might be shown the following clue:

"The average $\frac{x_1+x_2+\cdots+x_n}{n}$,"

to which she would reply "What is the maximum likelihood estimate for the mean of *n* independent identically distributed Gaussian random variables from which samples $x_1, x_2, \ldots, x_n$ have been obtained?" Host Alex Trebek would immediately exclaim "That is the correct answer for $200!"

The process of doing mathematics involves repeatedly playing ***Jeopardy!*** with oneself in an unending quest to understand everything just a little bit better. The purpose of this blog post is to provide an exposition of how this works for understanding principal component analysis (PCA): I present four Jeopardy clues in the "Normality" category that all share the same answer: "What is principal component analysis?" The post was motivated by a conversation I recently had with a well-known population geneticist at a conference I was attending. I mentioned to him that I would be saying something about PCA in my talk, and that he might find what I have to say interesting because I knew he had used the method in many of his papers. Without hesitation he replied that he was well aware that PCA was not a statistical method and merely a heuristic visualization tool.

The problem, of course, is that PCA does have a statistical interpretation and is not at all an ad-hoc heuristic. Unfortunately, the previously mentioned population geneticist is not alone; there is a lot of confusion about what PCA is really about. For example, in one textbook it is stated that "**PCA is not a statistical method** to infer parameters or test hypotheses. Instead, it provides a method to reduce a complex dataset to lower dimension to reveal sometimes hidden, simplified structure that often underlie it." In another one finds out that "**PCA is a statistical method** routinely used to analyze interrelationships among large numbers of objects." In a highly cited review on gene expression analysis PCA is described as "**more useful as a visualization technique than as an analytical method**" but then in a paper by Markus Ringnér titled the same as this post, i.e. What is principal component analysis? in *Nature Biotechnology*, 2008, the author writes that "**Principal component analysis (PCA) is a mathematical algorithm** that reduces the dimensionality of the data while retaining most of the variation in the data set" (the author then avoids going into the details because "understanding the details underlying PCA requires knowledge of linear algebra"). All of these statements are both correct and incorrect and confusing. A major issue is that the description by Ringnér of PCA in terms of the procedure for computing it (singular value decomposition) is common and unfortunately does not shed light on when it should be used. But knowing *when* to use a method is far more important than knowing *how* to do it.

I therefore offer four ***Jeopardy!*** clues for principal component analysis that I think help to understand both when and how to use the method:

1. An affine subspace closest to a set of points.

Suppose we are given *n* numbers $x_1, \ldots, x_n$ as in the initial example above. We are interested in finding the "closest" number to these numbers. By "closest" we mean in the sense of total squared difference. That is, we are looking for a number m such that $\sum_{i=1}^{n}(m - x_i)^2$ is minimized.

This is a (straightforward) calculus problem, solved by taking the derivative of the function above and setting it equal to zero. If we let $f(m) = \sum_{i=1}^{n}(m - x_i)^2$ then $f'(m) = 2 \cdot \sum_{i=1}^{n}(m - x_i)$ and setting $f'(m) = 0$ we can solve for m to obtain $m = \frac{1}{n}\sum_{i=1}^{n} x_i$.

The right hand side of the equation is just the average of the *n* numbers and the optimization problem provides an interpretation of it as the number minimizing the total squared difference with the given numbers (note that one can replace squared difference by absolute value, i.e. minimization of $\sum_{i=1}^{n} |m - x_i|$, in which case the solution for *m* is the median; we return to this point and its implications for PCA later).

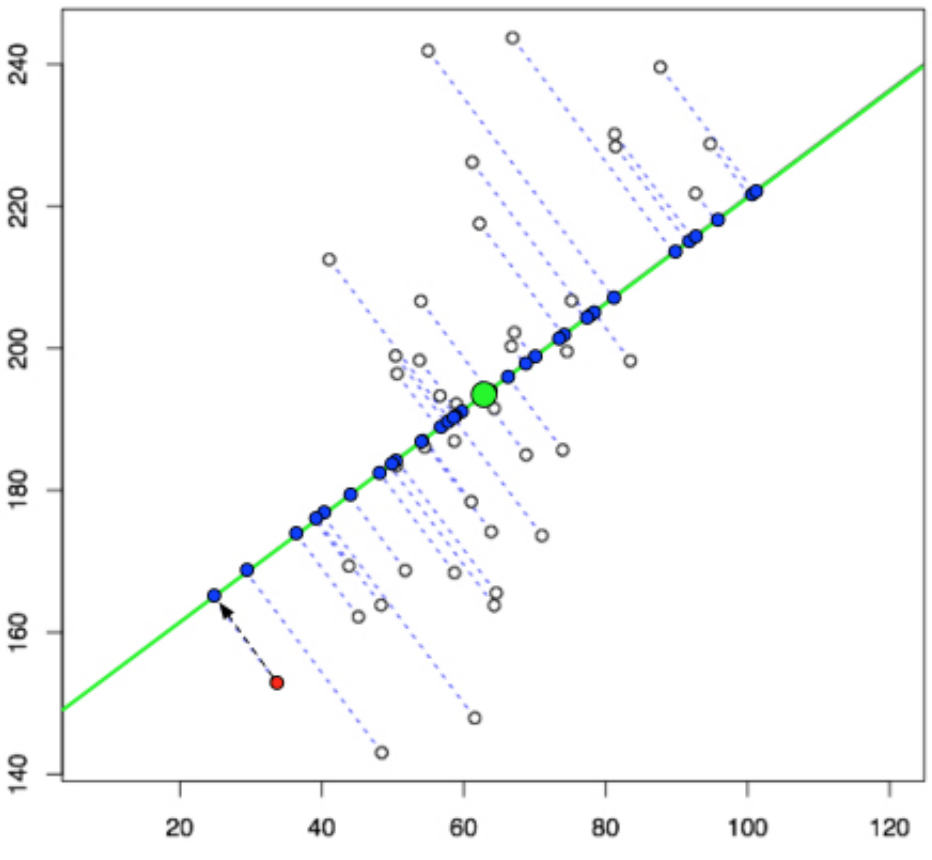
Suppose that instead of *n* numbers, one is given *n points* in $\mathbb{R}^p$. That is, point *i* is $\mathbf{x}^i = (x_1^i, \ldots, x_p^i)$. We can now ask for a point $\mathbf{m}$ with the property that the squared distance of $\mathbf{m}$ to the *n* points is minimized. This is asking for $min_{\mathbf{m}} \sum_{i=1}^{n} ||\mathbf{m} - \mathbf{x}^i||_2$.

The solution for m can be obtained by minimizing each coordinate independently, thereby reducing the problem to the simpler version of numbers above, and it follows that $\mathbf{m} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}^i$.

This is *0-dimensional PCA,* i.e., PCA of a set of points onto a single point, and it is the centroid of the points. The generalization of this concept provides a definition for PCA:

Definition: Given *n* points in $\mathbb{R}^p$, principal components analysis consists of choosing a dimension $k < p$ and then finding the affine space of dimension *k* with the property that the squared distance of the points to their orthogonal projection onto the space is minimized.

This definition can be thought of as a generalization of the centroid (or average) of the points. To understand this generalization, it is useful to think of the simplest case that is not 0-dimensional PCA, namely 1-dimensional PCA of a set of points in two dimensions:



In this case the 1-dimensional PCA subspace can be thought of as the *line* that best represents the average of the points. The blue points are the orthogonal projections of the points onto the "average line" (see, e.g., the red point projected orthogonally), which minimizes the squared lengths of the dashed lines. In higher dimensions line is replaced by affine subspace, and the orthogonal projections are to points on that subspace. There are a few properties of the PCA affine subspaces that are worth noting:

1. The set of PCA subspaces (translated to the origin) form a *flag*. This means that the PCA subspace of dimension *k* is contained in the PCA subspace of dimension *k+1*. For example, all PCA subspaces contain the centroid of the points (in the figure above the centroid is the green point). This follows from the fact that the PCA subspaces can be incrementally constructed by building a basis from eigenvectors of a single matrix, a point we will return to later.
2. The PCA subspaces are not scale invariant. For example, if the points are scaled by multiplying one of the coordinates by a constant, then the PCA subspaces change. This is obvious because the centroid of the points will change. For this reason, when PCA is applied to data obtained from heterogeneous measurements, the units matter. One can form a "common" set of units by scaling the values in each coordinate to have the same variance.
3. If the data points are represented in matrix form as an $n \times p$ matrix X, and the points orthogonally projected onto the PCA subspace of dimension *k* are represented as in the ambient *p* dimensional space by a matrix $\tilde{X}$, then $\tilde{X} = argmin_{M:rk(M)=k}||X - M||_2$. That is, $\tilde{X}$ is the matrix of rank *k* with the property that the Frobenius norm $||X - \tilde{X}||_2$ is minimized. This is just a rephrasing in linear algebra of the definition of PCA given above.

At this point it is useful to mention some terminology confusion associated with PCA. Unfortunately there is no standard for describing the various parts of an analysis. What I have called the "PCA subspaces" are also sometimes called "principal axes". The orthogonal vectors forming the flag mentioned above are called "weight vectors", or "loadings". Sometimes they are called "principal components", although that term is sometimes used to refer to points projected onto a principal axis. In this post I stick to "PCA subspaces" and "PCA points" to avoid confusion.

Returning to ***Jeopardy!***, we have "Normality for $400" with the answer "An affine subspace closest to a set of points" and the question "What is PCA?". One question at this point is why the ***Jeopardy!*** question just asked is in the category "Normality". After all, the normal distribution does not seem to be related to the optimization problem just discussed. The connection is as follows:

2. A generalization of linear regression in which the Gaussian noise is isotropic.

PCA has an interpretation as the maximum likelihood parameter of a linear Gaussian model, a point that is crucial in understanding the scope of its application. To explain this point of view, we begin by elaborating on the opening ***Jeopardy!*** question about Normality for $200:

The point of the question was that the average of *n* numbers can be interpreted as a maximum likelihood estimation of the mean of a Gaussian. The Gaussian distribution is

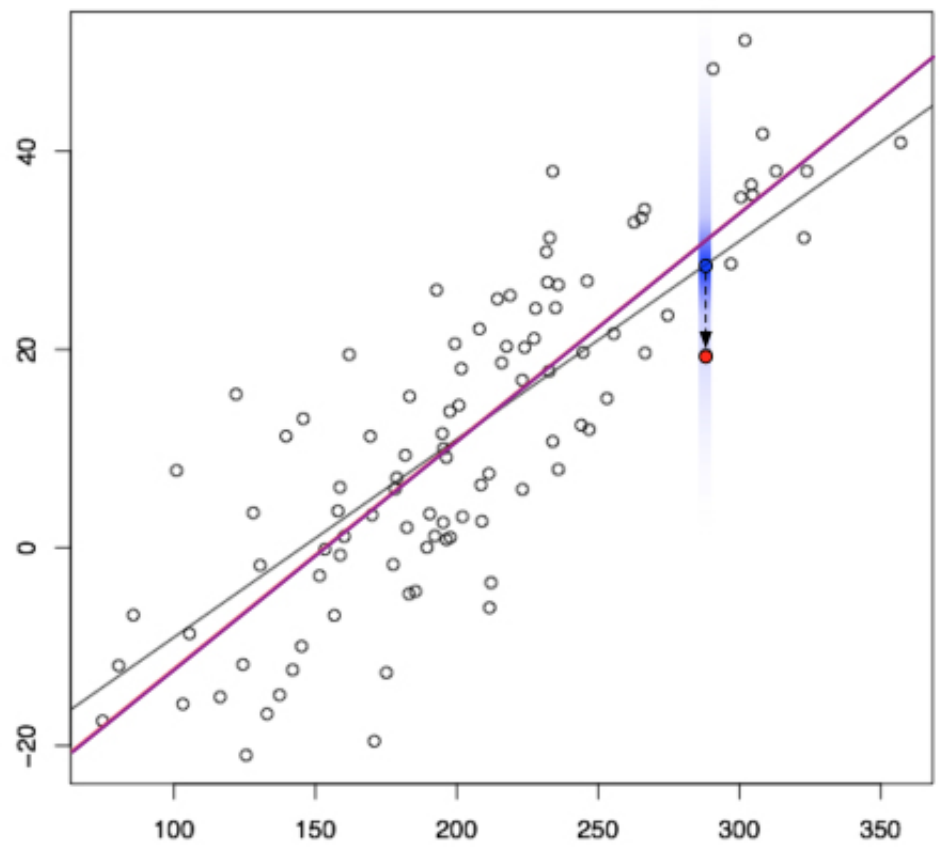
$f(x, \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$. Given the numbers $x_1, \ldots, x_n$, the likelihood function is therefore

$L(\mu, \sigma) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$. The maximum of this function is the same as the maximum of its logarithm, which is

$logL(\mu, \sigma) = \sum_{i=1}^{n} \left(log \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{(x_i-\mu)^2}{2\sigma^2} \right)$. Therefore the problem of finding the maximum likelihood estimate for the mean is equivalent to that of finding the *minimum* of the function

$S(\mu) = \sum_{i=1}^{n} (x_i - \mu)^2$. This is exactly the optimization problem solved by 0-dimensional PCA, as we saw above. With this

calculation at hand, we turn to the statistical interpretation of least squares:

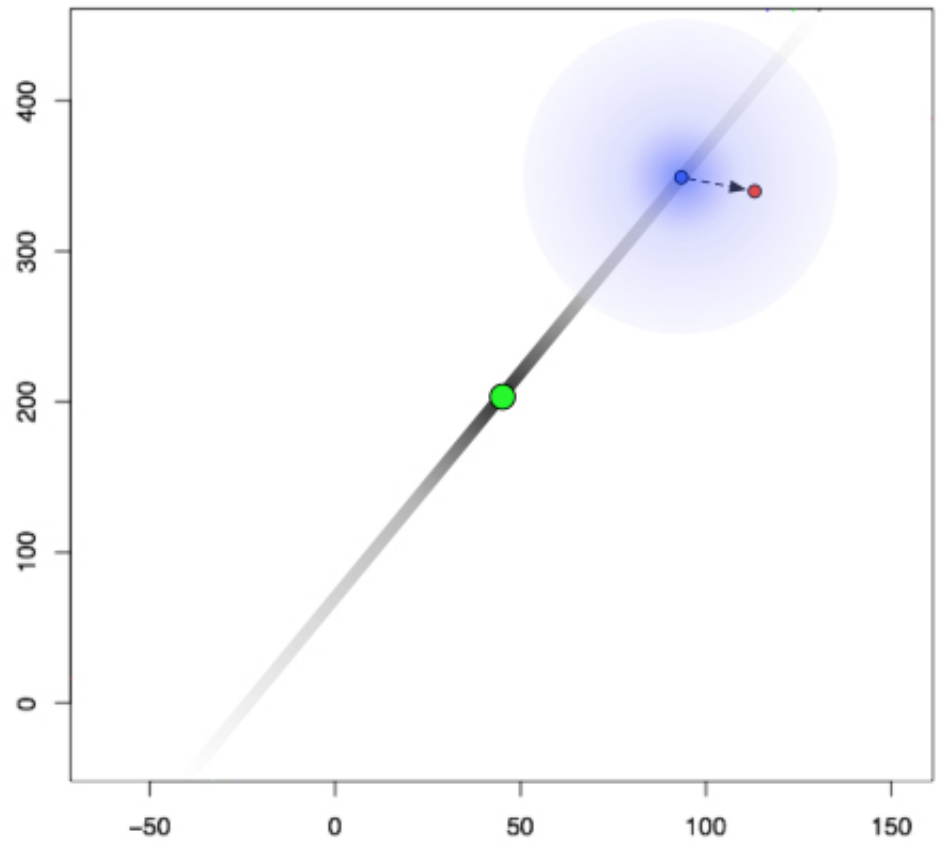


Given *n* points $\{(x_i, y_i)\}_{i=1}^n$ in the plane (see figure above), the least squares line $y = mx + b$ (purple in figure) is the one that minimizes the sum of the squares $\sum_{i=1}^n ((mx_i + b) - y_i)^2$. That is, the least squares line is the one minimizing the sum of the squared vertical distances to the points. As with the average of numbers, the least squares line has a statistical interpretation: Suppose that there is some line $y = m^*x + b^*$ (black line in figure) that is unknown, but that "generated" the observed points, in the sense that each observed point *i* was obtained by perturbing the point $m^*x_i + b^*$ vertically by a random amount from a single Gaussian distribution with mean 0 and variance σ^2. In the figure, an example is shown where the blue point on the unknown line "generates" the observed red point; the Gaussian is indicated with the blue streak around the point. Note that the model specified so far is not fully generative, as it depends on the hidden points $m^*x_i + b^*$ and there is no procedure given to generate the x_i. This can be done by positing that the x_i are generated from a Gaussian distribution along the line $y = m^*x + b$ (followed by the points y_i generated by Gaussian perturbation of the *y* coordinate on the line). The coordinates x_i can then be deduced directly from the observed points as the Gaussian perturbations are all vertical. The relationship between the statistical model just described and least squares is made precise by a theorem (which we state informally, but is a special case of the Gauss-Markov theorem):

Theorem (Gauss-Markov): The maximum likelihood estimate for the line (the parameters *m* and *b*) in the model described above correspond to the least squares line.

The proof is analogous to the argument given for the average of numbers above so we omit it. It can be generalized to higher dimensions where it forms the basis of what is known as linear regression. In regression, the x_i are known as independent variables and y the dependent variable. The generative model provides an interpretation of the independent variables as fixed measured quantities, whereas the dependent variable is a linear combination of the independent variables with added noise. It is important to note that the origins of linear regression are in physics, specifically in work of Legendre (1805) and Gauss (1809) who applied least squares to the astronomical problem of calculating the orbits of comets around the sun. In their application, the independent variables were time (for which accurate measurements were possible with clocks; by 1800 clocks were accurate to less than 0.15 seconds per day) and the (noisy) dependent variable the measurement of location. Linear regression has become one of the most (if not *the* most) widely used statistical tools but as we now explain, **PCA (and its generalization factor analysis), with a statistical interpretation that includes noise in the x_i variables, seems better suited for biological data.**

The statistical interpretation of least squares can be extended to a similar framework for PCA. Recall that we first considered a statistical interpretation for least squares where an unknown line $y = m^*x + b^*$ "generated" the observed points, in the sense that each observed point *i* was obtained by perturbing the point $m^*x_i + b^*$ *vertically* by a random amount from a single Gaussian distribution with mean 0 and variance σ^2. PCA can be understood analogously by replacing *vertically* by *orthogonally* (this is the probabilistic model of Collins *et al.*, NIPS 2001 for PCA). However this approach is not completely satisfactory as the orthogonality of the perturbation is is not readily interpretable. Stated differently, it is not obvious what physical processes would generate points orthogonal to a linear affine subspace by perturbations that are always orthogonal to the subspace. In the case of least squares, the "vertical" perturbation corresponds to noise in one measurement (represented by one coordinate). The problem is in naturally interpreting orthogonal perturbations in terms of a noise model for measurements. This difficulty is resolved by a model called *probabilistic PCA (pPCA),* first proposed by Tipping and Bishop in a Tech Report in 1997, and published in the J. of the Royal Statistical Society B 2002, and independently by Sam Roweis, NIPS 1998, that is illustrated visually in the figure below, and that we now explain:

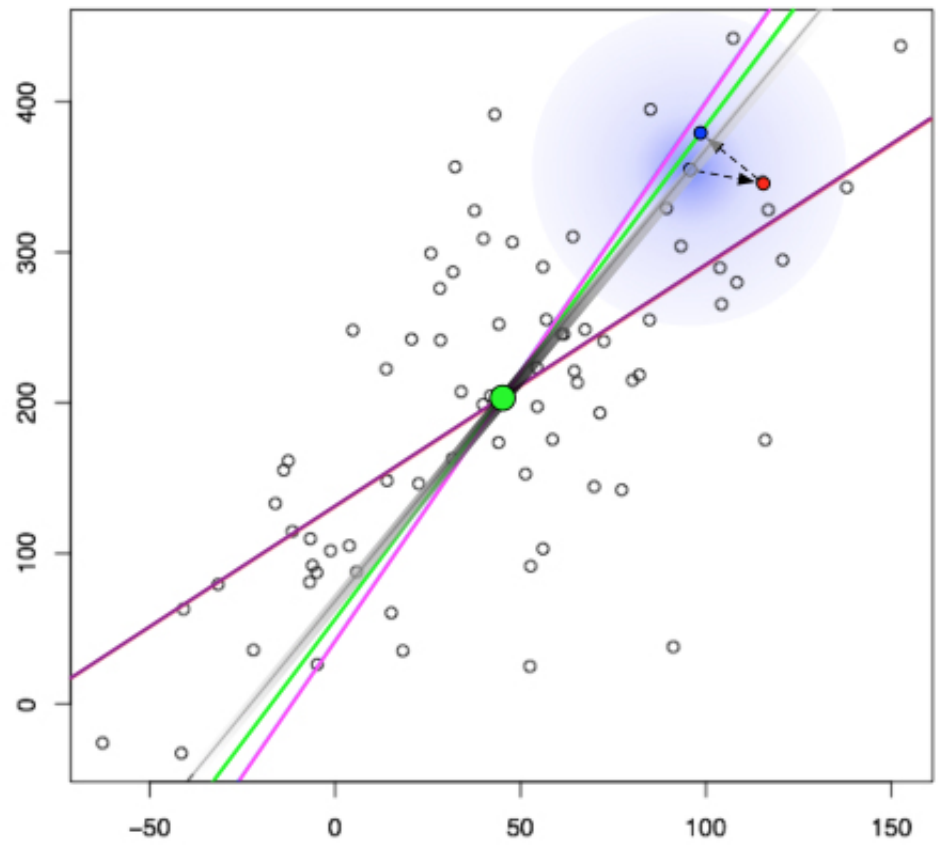


In the pPCA model there is an (unknown) line (affine space in higher dimension) on which (hidden) points (blue) are generated at random according to a Gaussian distribution (represented by gray streak in the figure above, where the mean of the Gaussian is the green point). Observed points (red) are then generated from the hidden points by addition of isotropic Gaussian noise (blue smear), meaning that the Gaussian has a diagonal covariance matrix with equal entries. Formally, in the notation of Tipping and Bishop, this is a linear Gaussian model described as follows:

Observed random variables *t* are given by $t = Wx + \mu + \epsilon$ where *x* are latent (hidden) random variables, *W* is a matrix describing a subspace and $Wx + \mu$ are the latent points on an affine subspace (μ corresponds to a translation). Finally, ϵ is an error term, given by a Gaussian random variable with mean 0 and covariance matrix $\sigma^2 I$. The parameters of the model are W, μ and σ^2. Equivalently, the observed random variables are themselves Gaussian, described by the distribution $t \sim \mathcal{N}(\mu, WW^T + \psi)$ where $\psi \sim \mathcal{N}(0, \sigma^2 I)$. Tipping and Bishop prove an analogy of the Gauss-Markov theorem, namely that the affine subspace given by the maximum likelihood estimates of W and μ is the PCA subspace (the proof is not difficult but I omit it and refer interested readers to their paper, or Bishop's Pattern Recognition and Machine Learning book).

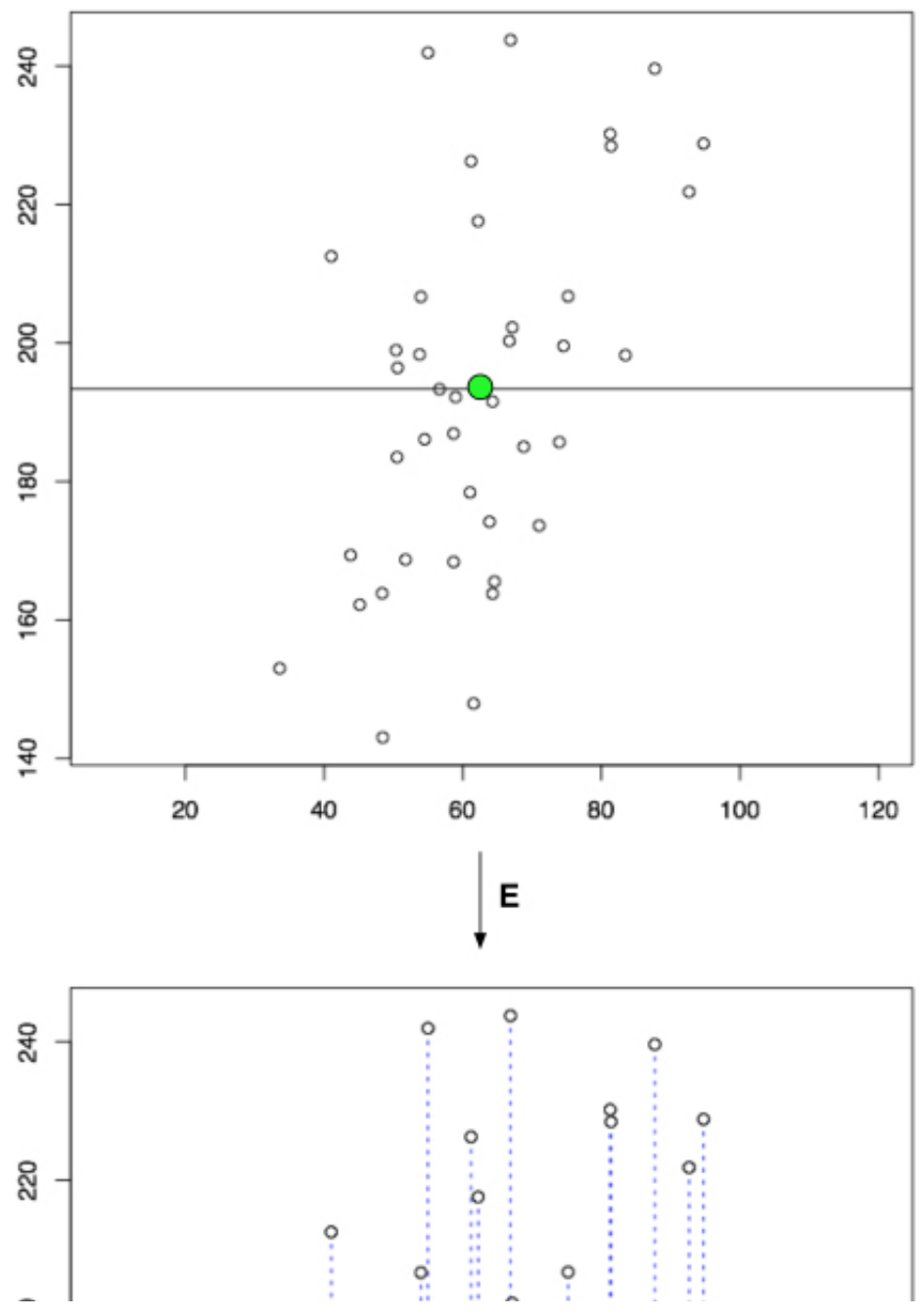
It is important to note that although the maximum likelihood estimates of W, μ in the pPCA model correspond to the PCA subspace, only posterior distributions can be obtained for the latent data (points on the subspace). Neither the mode nor the mean of those distributions corresponds to the PCA points (orthogonal projections of the observations onto the subspace). However what is true, is that the posterior distributions converge to the PCA points as $\sigma^2 \to 0$. In other words, the relationship between pPCA and PCA is a bit more subtle than that between least squares and regression.

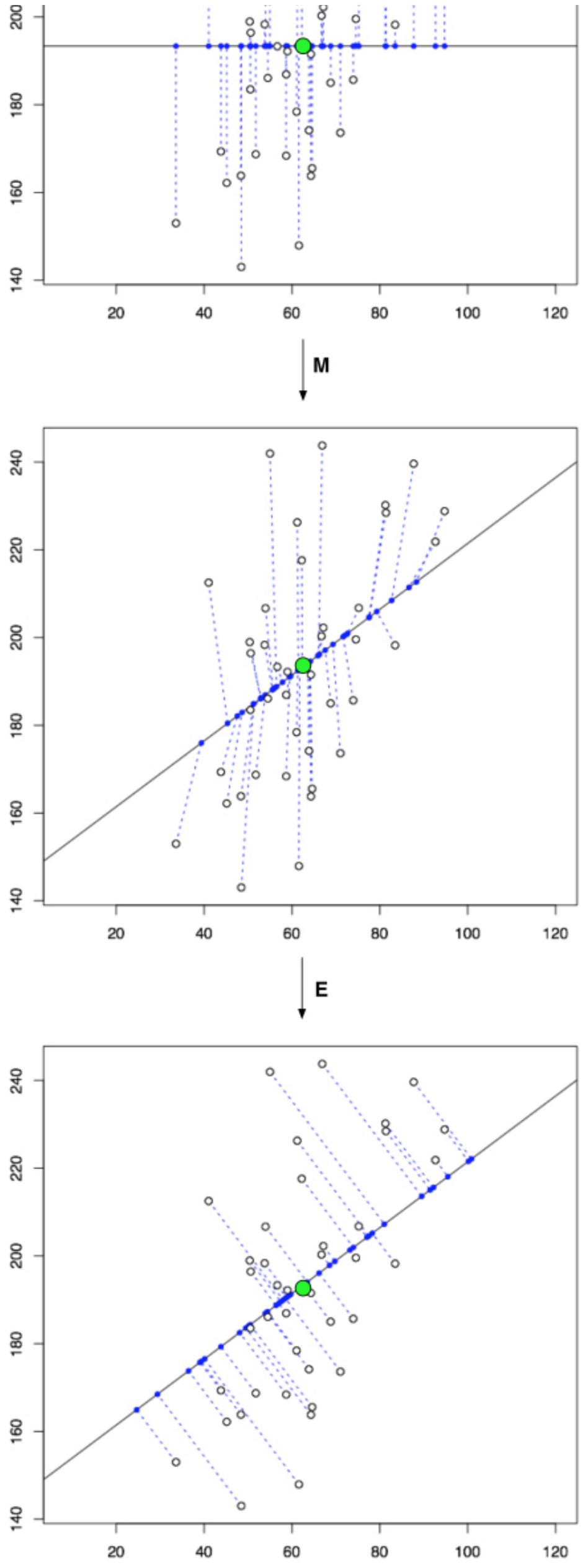
The relationship between regression and (p)PCA is shown in the figure below:



In the figure, points have been generated randomly according to the pPCA model. the black smear shows the affine space on which the points were generated, with the smear indicating the Gaussian distribution used. Subsequently the latent points (light blue on the gray line) were used to make observed points (red) by the addition of isotropic Gaussian noise. The green line is the maximum likelihood estimate for the space, or equivalently by the theorem of Tipping and Bishop the PCA subspace. The projection of the observed points onto the PCA subspace (blue) are the PCA points. The purple line is the least squares line, or equivalently the affine space obtained by regression (y observed as a noisy function of x). The pink line is also a regression line, except where x is observed as a noisy function of y.

A natural question to ask is why the probabilistic interpretation of PCA (pPCA) is useful or necessary? One reason it is beneficial is that maximum likelihood inference for pPCA involves hidden random variables, and therefore the EM algorithm immediately comes to mind as a solution (the strategy was suggested by both Tipping & Bishop and Roweis). I have not yet discussed *how* to find the PCA subspace, and the EM algorithm provides an intuitive and direct way to see how it can be done, without the need for writing down any linear algebra:





The exact version of the EM shown above is due to Roweis. In it, one begins with a random affine subspace passing through the centroid of the points. The “E” step (expectation) consists of projecting the points to the subspace. The projected points are considered fixed to the subspace. The “M” step (maximization) then consists of rotating the space so that the total squared distance of the fixed points on the subspace to the observed points is minimized. This is repeated until convergence. Roweis points out that this approach to finding the PCA subspace is equivalent to power iteration for (efficiently) finding eigenvalues of the the sample covariance matrix without computing it directly. This is our first use of the word eigenvalue in describing PCA, and we elaborate on it, and the linear algebra of computing PCA subspaces later in the post.

Another point of note is that pPCA can be viewed as a special case of factor analysis, and this connection provides an immediate starting point for thinking about generalizations of PCA. Specifically, factor analysis corresponds to the model $t \sim \mathcal{N}(\mu, WW^T + \psi)$

where the covariance matrix ψ is less constrained, and only required to be diagonal. This is connected to a comment made above about when the PCA subspace might be more useful as a linear fit to data than regression. To reiterate, unlike physics, where some coordinate measurements have very little noise in comparison to others, biological measurements are frequently noisy in all coordinates. In such settings factor analysis is preferable, as the variance in each coordinate is estimated as part of the model. PCA is perhaps a good compromise, as PCA subspaces are easier to find than parameters for factor analysis, yet PCA, via its pPCA interpretation, accounts for noise in all coordinates.

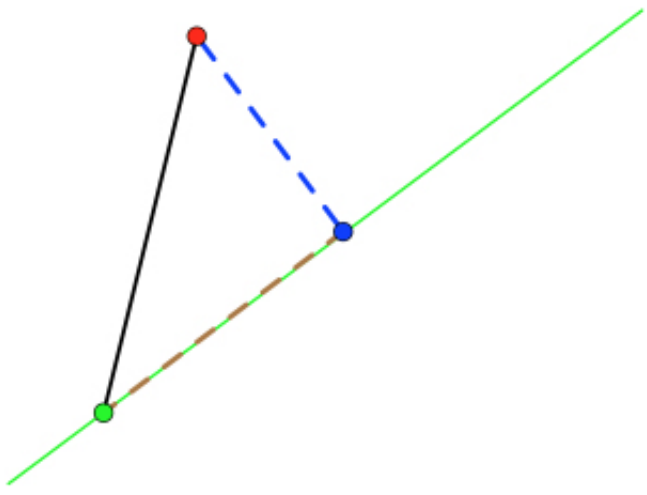
A final comment about pPCA is that it provides a natural framework for thinking about hypothesis testing. The book Statistical Methods: A Geometric Approach by Saville and Wood is essentially about (the geometry of) pPCA and its connection to hypothesis testing. The authors do not use the term pPCA but their starting point is exactly the linear Gaussian model of Tipping and Bishop. The idea is to consider single samples from *n* independent identically distributed independent Gaussian random variables as one single sample from a high-dimensional multivariate linear Gaussian model with isotropic noise. From that point of view pPCA provides an interpretation for Bessel's correction. The details are interesting but tangential to our focus on PCA.

We are therefore ready to return to ***Jeopardy!***, where we have "Normality for $600″ with the answer "A generalization of linear regression in which the Gaussian noise is isotropic" and the question "What is PCA?"

3. An orthogonal projection of points onto an affine space that maximizes the retained sample variance.

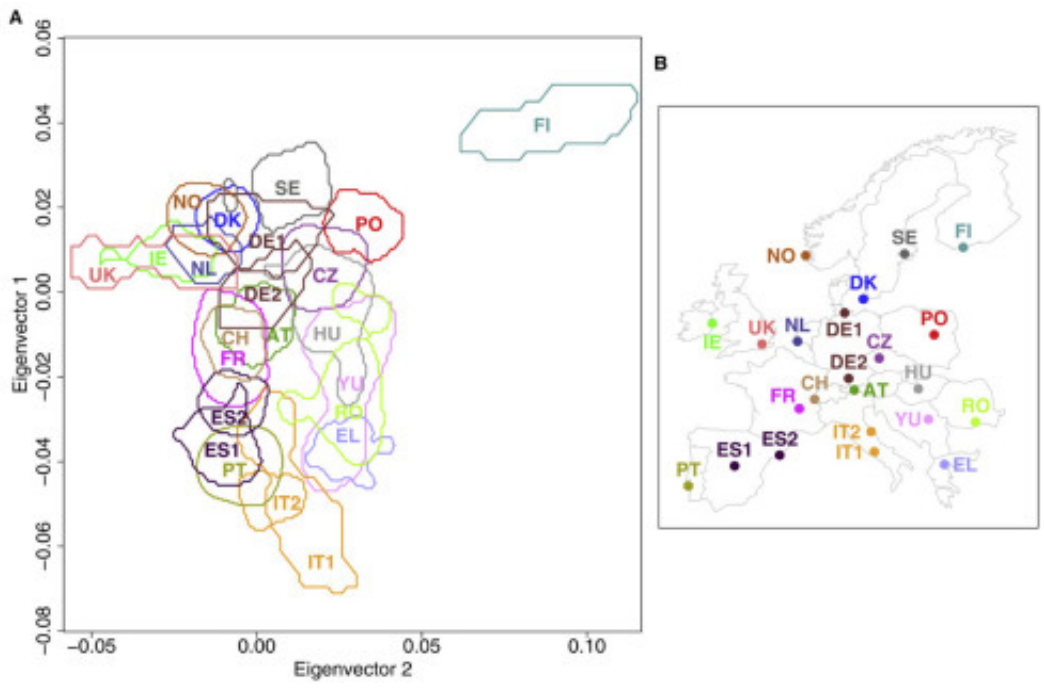
In the previous two interpretations of PCA, the focus was on the PCA affine subspace. However in many uses of PCA the output of interest is the *projection of the given points onto the PCA affine space*. The projected points have three useful related interpretations:

1. As seen in in section 1, the (orthogonally) projected points (red -> blue) are those whose total squared distance to the observed points is minimized.
2. What we focus on in this section, is the interpretation that the PCA subspace is the one onto which the (orthogonally) projected points maximize the retained sample variance.
3. The topic of the next section, namely that the squared distances between the (orthogonally) projected points are on average (in the l_2 metric) closest to the original distances between the points.



The *sample variance* of a set of points is the average squared distance from each point to the centroid. Mathematically, if the observed points are translated so that their centroid is at zero (known as zero-centering), and then represented by an $n \times p$ matrix *X*, then the sample covariance matrix is given by $\frac{1}{n-1}X^tX$ and the sample variance is given by the trace of the matrix. The point is that the *j*th diagonal entry of $\frac{1}{n-1}X^tX$ is just $\frac{1}{n-1}\sum_{i=1}^{n}(x_j^i)^2$, which is the sample variance of the *j*th variable. The PCA subspace can be viewed as that subspace with the property that *the sample variance of the projections of the observed points onto the subspace* is maximized. This is easy to see from the figure above. For each point (blue), Pythagoras' theorem implies that $d(red, blue)^2 + d(blue, green)^2 = d(red, green)^2$. Since the PCA subspace is the one minimizing the total squared red-blue distances, and since the solid black lines (red-green distances) are fixed, it follows that the PCA subspace also maximizes the total squared green-blue distances. In other words, PCA maximizes the retained sample variance.

The explanation above is informal, and uses a 1-dimensional PCA subspace in dimension 2 to make the argument. However the argument extends easily to higher dimension, which is typically the setting where PCA is used. In fact, PCA is typically used to "visualize" high dimensional points by projection into dimensions two or three, precisely because of the interpretation provided above, namely that it retains the sample variance. I put visualize in quotes because intuition in two or three dimensions does not always hold in high dimensions. However PCA can be useful for visualization, and one of my favorite examples is the evidence for genes mirroring geography in humans. This was first alluded to by Cavalli-Sforza, but definitively shown by Lao *et al.*, 2008, who analyzed 2541 individuals and showed that PCA of the SNP matrix (approximately) recapitulates geography:



Genes mirror geography from Lao *et al.* 2008: (Left) PCA of the SNP matrix (2541 individuals x 309,790 SNPs) showing a density map of projected points. (Right) Map of Europe showing locations of the populations .

In the picture above, it is useful to keep in mind that the emergence of geography is occurring in that projection in which the sample variance is maximized. As far as interpretation goes, it is useful to look back at Cavalli-Sforza's work. He and collaborators who worked on the problem in the 1970s, were unable to obtain a dense SNP matrix due to limited technology of the time. Instead, in Menozzi *et al.*, 1978 they performed PCA of an *allele-frequency* matrix, i.e. a matrix indexed by populations and allele frequencies instead of individuals and genotypes. Unfortunately they fell into the trap of misinterpreting the biological meaning of the eigenvectors in PCA. Specifically, they inferred migration patterns from contour plots in geographic space obtained by plotting the relative contributions from the eigenvectors, but the effects they observed turned out to be an artifact of PCA. However as we discussed above, PCA *can* be used quantitatively via the stochastic process for which it solves maximum likelihood inference. It just has to be properly understood.

To conclude this section in ***Jeopardy!*** language, we have "Normality for $800″ with the answer "A set of points in an affine space obtained via projection of a set of given points so that the sample variance of the projected points is maximized" and the question "What is PCA?"

4. Principal component analysis of Euclidean distance matrices.

In the preceding interpretations of PCA, I have focused on what happens to individual points when projected to a lower dimensional subspace, but it is also interesting to consider what happens to *pairs* of points. One thing that is clear is that if a pair of points are projected orthogonally onto a low-dimensional affine subspace then the distance between the points in the projection is smaller than the original distance between the points. This is clear because of Pythagoras' theorem, which implies that the squared distance will shrink unless the points are parallel to the subspace in which case the distance remains the same. An interesting observation is that in fact the PCA subspace is the one with the property where the average (or total) squared distances between the points is maximized. To see this it again suffices to consider only projections onto one dimension (the general case follows by Pythagoras' theorem). The following lemma, discussed in my previous blog post, makes the connection to the previous discussion:

Lemma: Let $x_1, \ldots, x_n$ be numbers with mean $\overline{x} = \frac{1}{n}\sum_i x_i$. If the average squared distance between pairs of points is denoted $D = \frac{1}{n^2}\sum_{i,j}(x_i - x_j)^2$ and the variance is denoted $V = \frac{1}{n}\sum_i (x_i - \overline{x})^2$ then $V = \frac{1}{2}D$.

What the lemma says is that the sample variance is equal to the average squared difference between the numbers (i.e. it is a scalar multiple that does not depend on the numbers). I have already discussed that the PCA subspace maximizes the retained variance, and it therefore follows that it also maximizes the average (or total) projected squared distance between the points. Alternately, PCA can be interpreted as *minimizing* the total (squared) distance that is lost, i,e. if the original distances between the points are given by a distance matrix D and the projected distances are given by $\tilde{D}$, then the PCA subspace minimizes $\sum_{ij}(D_{ij}^2 - \tilde{D}_{ij}^2)$, where each term in the sum is positive as discussed above.

This interpretation of PCA leads to an interesting application of the method to (Euclidean) *distance matrices* rather than *points.* The idea is based on a theorem of Isaac Schoenberg that characterizes Euclidean distance matrices and provides a method for realizing them. The theorem is well-known to structural biologists who work with NMR, because it is one of the foundations used to reconstruct coordinates of structures from distance measurements. It requires a bit of notation: *D* is a distance matrix with entries d_{ij} and Δ is the matrix with entries $-\frac{1}{2}d_{ij}^2$. $\mathbf{1}$ denotes the vector of all ones, and $\mathbf{s}$ denotes a vector.

Theorem (Schoenberg, 1938): A matrix *D* is a Euclidean distance matrix if and only if the matrix $B = (I - \mathbf{1s}')\Delta(I - \mathbf{s1}')$ is positive semi-definite where $\mathbf{s}'\mathbf{1} = 1$.

For the case when $\mathbf{s}$ is chosen to be a unit vector, i.e. all entries are zero except one of them equal to 1, the matrix *B* can be viewed as the Gromov transform (known as the Farris transform in phylogenetics) of the matrix with entries d_{ij}^2. Since the matrix *B* is positive semidefinite it can be written as $B = XX^t$, where the matrix *X* provides coordinates for points that realize *D.* At this point PCA can be applied resulting in a principal subspace and points on it (the orthogonal projections of *X).* A point of note is that eigenvectors of XX^t can be computed directly, avoiding the need to compute X^tX which may be a larger matrix if $n < p$.

The procedure just described is called classic multidimensional scaling (MDS) and it returns a set of points on a Euclidean subspace with distance matrix $\tilde{D}$ that best represent the original distance matrix D in the sense that $\sum_{ij}(D_{ij}^2 - \tilde{D}_{ij}^2)$ is minimized. The term multidimensional scaling without the "classic" has taken on an expanded meaning, namely it encapsulates all methods that seek to approximately realize a distance matrix by points in a low dimensional Euclidean space. Such methods are generally not related to PCA, but classic multidimensional scaling *is* PCA. This is a general source of confusion and error on the internet. In fact, most articles and course notes I found online describing the connection between MDS and PCA are incorrect. In any case classic multidimensional scaling is a very useful instance of PCA, because it extends the utility of the method to cases where points are not available but distances between them are.

Now we return to ***Jeopardy!*** one final time with the final question in the category: "Normality for $1000″. The answer is "Principal component analysis of Euclidean distance matrices" and the question is "What is classic multidimensional scaling?"

An example

To illustrate the interpretations of PCA I have highlighted, I'm including an example in R inspired by an example from another blog post (all commands can be directly pasted into an R console). I'm also providing the example because missing in the discussion above is a description of *how* to compute PCA subspaces and the projections of points onto them. I therefore explain some of this math in the course of working out the example:

First, I generate a set of points (in $\mathbb{R}^2$). I've chosen a low dimension so that pictures can be drawn that are compatible with some of the examples above. Comments following commands appear after the # character.

```
set.seed(2)                 #sets the seed for random number generation.
x <- 1:100                  #creates a vector x with numbers from 1 to 100
ex <- rnorm(100, 0, 30) #100 normally distributed rand. nos. w/ mean=0, s.d.=30
ey <- rnorm(100, 0, 30) # " "
y <- 30 + 2 * x             #sets y to be a vector that is a linear function of x
x_obs <- x + ex             #adds "noise" to x
y_obs <- y + ey             #adds "noise" to y
P <- cbind(x_obs,y_obs) #places points in matrix
plot(P,asp=1,col=1) #plot points
points(mean(x_obs),mean(y_obs),col=3, pch=19) #show center
```

At this point a full PCA analysis can be undertaken in R using the command "prcomp", but in order to illustrate the algorithm I show all the steps below:

```
M <- cbind(x_obs-mean(x_obs),y_obs-mean(y_obs))#centered matrix
MCov <- cov(M)              #creates covariance matrix
```

Note that the covariance matrix is proportional to the matrix M^tM. Next I turn to computation of the principal axes:

```
eigenValues <- eigen(MCov)$values       #compute eigenvalues
eigenVectors <- eigen(MCov)$vectors     #compute eigenvectors
```

The eigenvectors of the covariance matrix provide the principal axes, and the eigenvalues quantify the fraction of variance explained in each component. This math is explained in many papers and books so we omit it here, except to say that the fact that eigenvalues of the sample covariance matrix are the principal axes follows from recasting the PCA optimization problem as maximization of the Raleigh quotient. A key point is that although I've computed the sample covariance matrix explicitly in this example, it is not necessary to do so in practice in order to obtain its eigenvectors. In fact, it is inadvisable to do so. Instead, it is computationally more efficient, and also more stable to directly compute the singular value decomposition of M. The singular value decomposition of M decomposes it into $M = UDV^t$ where D is a diagonal matrix and both U and V^t are orthogonal matrices. I will also not explain in detail the linear algebra of singular value decomposition and its relationship to eigenvectors of the sample covariance matrix (there is plenty of material elsewhere), and only show how to compute it in R:

```
d <- svd(M)$d               #the singular values
v <- svd(M)$v               #the right singular vectors
```

The right singular vectors are the eigenvectors of M^tM. Next I plot the principal axes:

```
lines(x_obs,eigenVectors[2,1]/eigenVectors[1,1]*M[x]+mean(y_obs),col=8)
```

This shows the first principal axis. Note that it passes through the mean as expected. The ratio of the eigenvectors gives the slope of the axis. Next

```
lines(x_obs,eigenVectors[2,2]/eigenVectors[1,2]*M[x]+mean(y_obs),col=8)
```

shows the second principal axis, which is orthogonal to the first (recall that the matrix V^t in the singular value decomposition is orthogonal). This can be checked by noting that the second principal axis is also

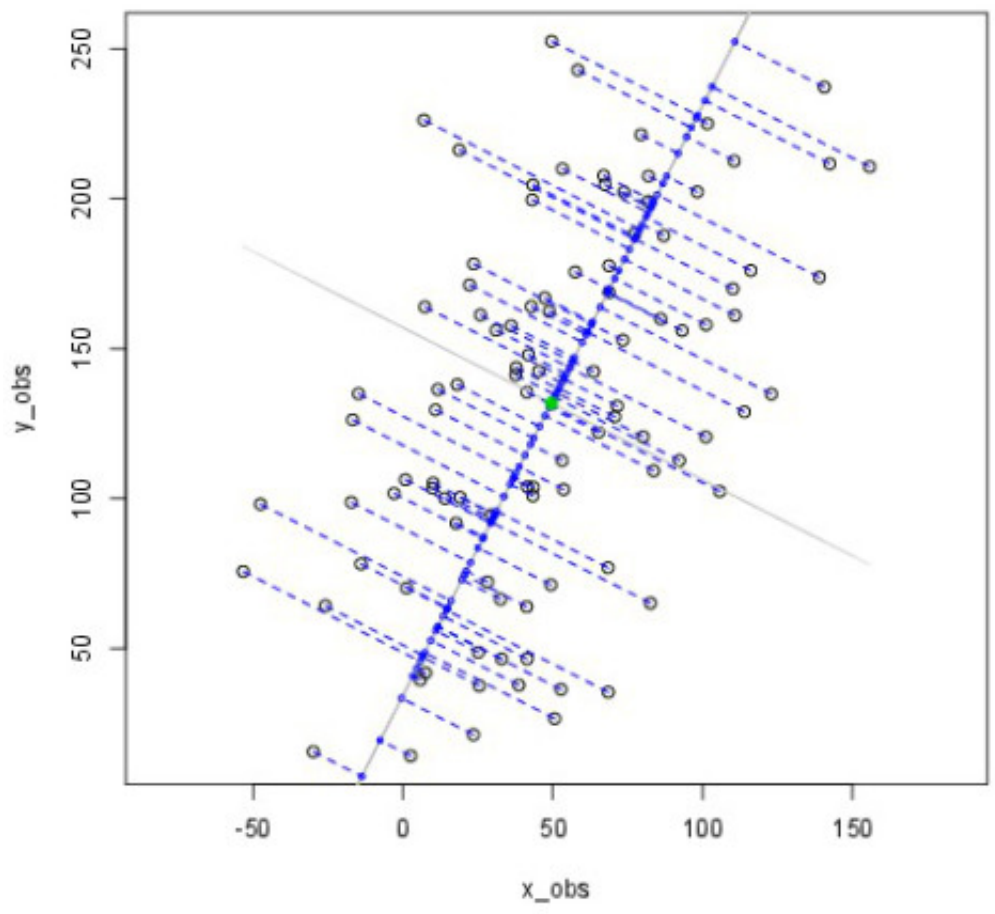
```
lines(x_obs,-1/(eigenVectors[2,1]/eigenVectors[1,1])*M[x]+mean(y_obs),col=8)
```

as the product of orthogonal slopes is -1. Next, I plot the projections of the points onto the first principal component:

```
trans <- (M%*%v[,1])%*%v[,1] #compute projections of points
P_proj <- scale(trans, center=-cbind(mean(x_obs),mean(y_obs)), scale=FALSE)
```

```
points(P_proj, col=4,pch=19,cex=0.5) #plot projections
segments(x_obs,y_obs,P_proj[,1],P_proj[,2],col=4,lty=2) #connect to points
```

The linear algebra of the projection is simply a rotation followed by a projection (and an extra step to recenter to the coordinates of the original points). Formally, the matrix *M* of points is rotated by the matrix of eigenvectors *W* to produce $T = MW$. This is the rotation that has all the optimality properties described above. The matrix *T* is sometimes called the PCA score matrix. All of the above code produces the following figure, which should be compared to those shown above:



There are many generalizations and modifications to PCA that go far beyond what has been presented here. The first step in generalizing probabilistic PCA is factor analysis, which includes estimation of variance parameters in each coordinate. Since it is rare that "noise" in data will be the same in each coordinate, factor analysis is almost always a better idea than PCA (although the numerical algorithms are more complicated). In other words, I just explained PCA in detail, now I'm saying don't use it! There are other aspects that have been generalized and extended. For example the Gaussian assumption can be relaxed to other members of the exponential family, an important idea if the data is discrete (as in genetics). Yang *et al.* 2012 exploit this idea by replacing PCA with logistic PCA for analysis of genotypes. There are also many constrained and regularized versions of PCA, all improving on the basic algorithm to deal with numerous issues and difficulties. Perhaps more importantly, there are issues in *using* PCA that I have not discussed. A big one is how to choose the PCA dimension to project to in analysis of high-dimensional data. But I am stopping here as I am certain no one is reading at this far into the post anyway…

The take-home message about PCA? Always be thinking when using it!

Acknowledgment: The exposition of PCA in this post began with notes I compiled for my course MCB/Math 239: 14 Lessons in Computational Genomics taught in the Spring of 2013. I thank students in that class for their questions and feedback. None of the material presented in class was new, but the exposition was intended to clarify when PCA ought to be used, and how. I was inspired by the papers of Tipping, Bishop and Roweis on probabilistic PCA in the late 1990s that provided the needed statistical framework for its understanding. Following the class I taught, I benefited greatly from conversations with Nicolas Bray, Brielin Brown, Isaac Joseph and Shannon McCurdy who helped me to further frame PCA in the way presented in this post.